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Abstract

We discuss the mathematical basis of sampling diffusive paths in Monte Carlo using Green's functions that are themselves built up stochastically from Green's functions in geometrical subdomains. The method of spheres is a special case. We show that other subdomains can be used as well, and may be more efficient for some applications. We include the basis for construction of such subdomain Green's functions for rectangular domains (in any number of dimensions) and cylindrical domains.

I. INTRODUCTION

Sampling diffusive paths in complicated geometries has a number of diverse applications. It arises in problems of heat conduction which may be treated by Monte Carlo, in the diffusion of radiation or chemical species, and in quantum Monte Carlo, especially in the computation of hard-sphere systems [1]. While there are rather straightforward approximate methods available, we will be concerned with exact and efficient methods that rely on the recursive stochastic generation that invoke integrals equations for Green's functions.

We consider the diffusion equation with a spatially dependent absorption rate $A(\vec{R}) > 0$ and a source of particles that emits $Q(\vec{R},t)$ per unit time at time t and position $\vec{R} \in \Omega$ in which the solution $\rho(\vec{R},t)$ is to be found.

$$[-\nabla^2 + A(\vec{R}) + \frac{\partial}{\partial t}]\rho(\vec{R},t) = Q(\vec{R},t). \tag{1.1}$$

Green's function for this equation is the solution of

$$\begin{aligned} [-\nabla^2 + A(\vec{R}) + \frac{\partial}{\partial t}]G(\vec{R},\vec{R}_0;t) &= 0; \qquad \vec{R},\vec{R}_0 \in \Omega \\ G(\vec{R},\vec{R}_0;0) &= \delta(\vec{R}-\vec{R}_0). \\ G(\vec{R},\vec{R}_0;t) &= 0; \qquad \vec{R},\vec{R}_0 \notin \Omega. \end{aligned} \tag{1.2}$$

A formal solution of Eq (1.1) that uses $G(\vec{R},\vec{R}_0;t)$ is

$$\rho(\vec{R},t) = \int_0^\infty \int_\Omega G(\vec{R},\vec{R}';t-t')Q(\vec{R}',t')d\vec{R}'dt. \tag{1.3}$$

If $G(\vec{R},\vec{R}_0;t)$ were known analytically, then Eq (1.3) would permit an analytic solution for some forms of $Q(\vec{R},t)$. Alternatively, if a method for sampling $G(\vec{R},\vec{R}_0;t)$ can be found, then

one may sample a time t' and a position $\vec{R}'$ from the function $Q(\vec{R}', t')$ and then, conditional on those coordinates, sample t and $\vec{R}$ from $G(\vec{R}, \vec{R}'; t - t')$. Unfortunately, except for some special cases, G is not generally known in interesting geometries. Our procedure can be considered as a method for sampling G in a recursive way, so that the second of the two possibilities can be carried through.

II. RECURSIVE COMPUTATION OF G

Divide the space Ω into two parts, Ω_0, and the complement, Ω_1 so that $\Omega = \Omega_0 \bigcup \Omega_1$. The boundary of Ω_0 is denoted by $\partial\Omega_0$. A diffusing object (which we will call a "walker") that starts at $\vec{R}_0 \in \partial\Omega_0$ must cross $\partial\Omega_0$ if it is to arrive at some position in Ω_1. We label the walkers in two ways distinguishing those that have not yet crossed $\partial\Omega_0$ from those that have. The property of "not yet crossed" or "NYC" is lost at the boundary, so that walkers labeled NYC are absorbed at the boundary (and then reemitted as the other kind of walker that can diffuse anywhere including back into Ω_0.) Let $G_0(\vec{R}, \vec{R}_0, t)$ be the distribution of the NYC walkers; it satisfies:

$$\begin{aligned} [-\nabla^2 + A(\vec{R}) + \frac{\partial}{\partial t}]G_0(\vec{R}, \vec{R}_0; t) &= 0; \qquad \vec{R}, \vec{R}_0 \in \Omega_0; \\ G_0(\vec{R}, \vec{R}_0; 0) &= \delta(\vec{R} - \vec{R}_0); \\ G_0(\vec{R}, \vec{R}_0; t) &= 0; \qquad \vec{R}, \vec{R}_0 \notin \Omega. \end{aligned} \tag{2.1}$$

Integrating Eq (2.1) over Ω_0 and using Green's theorem, we find that

$$\int_0^\infty \int_{\Omega_0} A(\vec{R}) G_0(\vec{R}, \vec{R}_0; t) d\vec{R} dt + \int_0^\infty \int_{\partial\Omega_0} [-\vec{n} \cdot \vec{\nabla} G_0(\vec{R}, \vec{R}_0; t)] \vec{R} dt = 1. \tag{2.2}$$

Here, $\vec{n}$ is a unit vector outer normal to $\partial\Omega_0$.

The first term of the last equation is clearly the net absorption of NYC walkers and the second term gives their net leakage across the boundary, $\partial\Omega_0$. Thus we may interpret the expression $-\vec{n} \cdot \vec{\nabla} G_0(\vec{R}, \vec{R}_0; t)$, the outer normal derivative of G_0 as the current of walkers that arrive at the boundary at position $\vec{R}$ and time t given that they were born at $\vec{R}_0$ at time zero.

Since the NYC walkers do in fact continue to diffuse after reaching the boundary of Ω_0, we may correctly regard the leakage current as a source for future diffusion. On that basis, and using Eq (1.3) we immediately conclude that

$$G(\vec{R}, \vec{R}_0; t) = G_0(\vec{R}, \vec{R}_0; t) + \int_0^t \int_{\partial\Omega_0} G(\vec{R}, \vec{R}'; t - t')[-\vec{n} \cdot \vec{\nabla} G_0(\vec{R}', \vec{R}_0; t')] d\vec{R} dt' \tag{2.3}$$

This equation may also be proved in a more formal way by multiplying Eq (1.2) by $G_0(\vec{R}, \vec{R}_0; t)$, Eq (2.1) by $G(\vec{R}, \vec{R}_0; t)$ subtracting, integrating, and again using Green's theorem.

In fact, solving Eq (2.1) is no easier than solving (1.2) so that the relation in Eq (2.3), while correct, is of no practical use. But we may proceed as follows. For every point $\vec{R}_k$ in Ω associate a domain Ω_k. Let U_k be an upper bound to the function $A(\vec{R})$ on Ω_k. That is

$$U_k \geq A(\vec{R}) \qquad \forall \vec{R} \in \Omega_k. \tag{2.4}$$

Now define a new Green's function in which U_k is the absorption rate:

$$\begin{aligned} [-\nabla^2 + U_k + \frac{\partial}{\partial t}]G_k(\vec{R}, \vec{R}_k; t) &= 0; \qquad \vec{R}, \vec{R}_k \in \Omega_k; \\ G_k(\vec{R}, \vec{R}_k; 0) &= \delta(\vec{R} - \vec{R}_k); \\ G_k(\vec{R}, \vec{R}_k; t) &= 0; \qquad \vec{R}, \vec{R}_k \notin \Omega. \end{aligned} \tag{2.5}$$

As we will see presently, there are useful classes of domains for which $G_k(\vec{R}, \vec{R}_k; t)$ satisfying Eq (2.5) can be found analytically, and to sample in the Monte Carlo sense. They overestimate the rate of absorption, but that is easy to correct: Walkers are absorbed at $\vec{R}$ in Ω_k at a rate $U_k G_k(\vec{R}, \vec{R}_k; t)$. If with probability $[U_k - A(\vec{R})]/U_k \geq 0$ the walkers are reemitted after an artificial absorption at $\vec{R}$, then the true absorption rate is exactly right. These reemitted walkers are also source particles for future diffusion so that the full recursion for $G(\vec{R}, \vec{R}_k; t)$ is now

$$\begin{aligned} G(\vec{R}, \vec{R}_k; t) = G_k(\vec{R}, \vec{R}_k; t) &+ \int_0^t \int_{\partial\Omega_k} G(\vec{R}, \vec{R}'; t - t')[-\vec{n} \cdot \vec{\nabla} G_k(\vec{R}', \vec{R}_k; t')d\vec{R}'dt' \\ &+ \int_0^t \int_{\Omega_k} G(\vec{R}, \vec{R}'; t - t')\frac{U_k - A(\vec{R}')}{U_k} U_k G_k(\vec{R}', \vec{R}_k; t')d\vec{R}'dt'. \end{aligned} \tag{2.6}$$

This equation may be derived more formally as indicated above for Eq (2.3), and may be verified by operating term by term on both sides with

$$-\nabla^2 + A(\vec{R}) + \frac{\partial}{\partial t} \equiv -\nabla^2 + U_k + [A(\vec{R}) - U_k] + \frac{\partial}{\partial t} \tag{2.7}$$

III. RANDOM WALKS AND INTEGRAL EQUATIONS

We now digress to establish the relationship of random walks and the kind of recursions for the Green's functions that we have developed.

Let $T(X|Y)$ be a stochastic kernel. That is, it satisfies

$$\begin{aligned} T(X|Y) &\geq 0 \\ \int T(X|Y)dX &\leq 1 \qquad \forall Y \end{aligned} \tag{3.1}$$

and the smallest eigenvalue λ_0 of T defined by

$$\varphi_m(X) = \lambda_m \int T(X|Y)\varphi_m(Y)dY \tag{3.2}$$

satisfies

$$\lambda_0 > 0 \tag{3.3}$$

Now let a random walk be defined by the sequence of steps $(Y, X_1, X_2, \cdots)$ chosen as follows:

$$\begin{aligned} X_1 &\text{ is sampled from } T(X_1|Y) \text{ conditional on } Y \\ X_2 &\text{ is sampled from } T(X_2|X_1) \text{ conditional on } X_1 \qquad \cdots \\ X_m &\text{ is sampled from } T(X_m|X_{m-1}) \text{ conditional on } X_{m-1} \end{aligned} \tag{3.4}$$

Define $K_m(Z|Y)$ to be the density of arrivals of walkers near Z after exactly m steps starting from Y following 3.4. Then

$$\begin{aligned} K_1(Z,Y) &= T(Z|Y) \\ K_2(Z,Y) &= \int T(Z|X)T(X|Y)dX \qquad \cdots \end{aligned} \tag{3.5}$$

$$\begin{aligned} K_m(Z|Y) &= \int \cdots \int T(Z|X_{m-1})T(X_{m-1}|X_{m-2}) \cdots T(X_1|Y)dX_1 \cdots dX_{m-1} \\ &= \int K_{m-1}(Z|X)T(X|Y)dX \end{aligned} \tag{3.6}$$

Let $K(Z|Y)$ be the the density of arrivals of walkers near Z after any number of steps. It is simply

$$K(Z|Y) = \sum_1^\infty K_m(Z|Y) \tag{3.7}$$

But

$$\int K(Z|X)T(X|Z)dX = \sum_2^\infty K_m(Z|Y) = K(Z|Y) - K_1(Z|Y), \tag{3.8}$$

or simply

$$\begin{aligned} \int K(Z|X)T(X|Y)dX &= \sum_2^\infty K_m(Z|Y) \\ &= K(Z|Y) - K_1(Z|Y); \\ K(Z|Y) &= T(Z|Y) + \int K(Z|X)T(X|Y)dX \end{aligned} \tag{3.9}$$

That is, the density of arrivals near Z is the sum of the density in exactly one step (given by $T(Z|Y) = K_1(Z|Y)$) plus the contribution of walks that go from Y to X in one step and then from X to Z in any additional number of steps, integrating over the intermediate position, X.

The recursive equation for the diffusive Green's function, Eq (2.6) has the structure of the last equation (noting, however, that its kernel has two parts corresponding to leakage across the surface and to absorption.) Thus we may construct a random walk that samples $G(\vec{R}, \vec{R}_0; t)$ by a random walk in which $-\vec{n} \cdot \vec{\nabla} G_k(\vec{R}', \vec{R}_k; t')$ or $U_k G_k(\vec{R}', \vec{R}_0; t')$ are sampled for successive positions.

IV. SAMPLING THE GREEN'S FUNCTION

The essence of the procedure is that at every stage, the walker is at some position $\vec{R}_k$. We select some subdomain Ω_k with $\vec{R}_k \in \Omega_k \subset \Omega$. In general Ω_k will be a member of some class of domains (spheres, rectangular parallelepipeds, cylindrical annuli, etc.) and we will select the largest that fits inside Ω. Given Ω_k, we construct $G_k(\vec{R}, \vec{R}_k; t)$ and sample it for a point of artificial absorption inside Ω_k or for a point on $\partial\Omega_0$ at which a walker escapes. At each step of the walk, a partial contribution to the full $G(\vec{R}, \vec{R}_0; t)$ is available, namely $G_k(\vec{R}, \vec{R}_0; t)$. We may use that to evaluate partial contributions to integrals over the full solution, or to generate random positions drawn from $G(\vec{R}, \vec{R}_0; t)$.

The details of the random walk are outlined below:

(1) Initialize:

$$k \leftarrow 0; \qquad t_k \leftarrow 0; \qquad \vec{R}_k \leftarrow \vec{R}_0; \qquad \Omega_k \leftarrow \Omega_0 \tag{4.1}$$

(2) Use $G_k(\vec{R}, \vec{R}_0; t)$ as contribution to $G(\vec{R}, \vec{R}_0; t)$.
(3) Sample $(\vec{R}_{k+1}, t_{k+1})$ from either
  (3.1) $U_k G_k(\vec{R}_{k+1}, \vec{R}_k; t_{k+1} - t_k)$ and then
    (3.11) Continue walk with probability $1 - A(\vec{R}_{k+1})/U_k$
    or else
    (3.12) terminate the walk;
  or else sample next $(\vec{R}_{k+1}, t_{k+1})$ from
  (3.2) $-\vec{n} \cdot \vec{\nabla} G_k(\vec{R}_{k+1}, \vec{R}_k; t_{k+1} - t_k)$ on $\partial\Omega_k$; if $\vec{R}_{k+1} \in \partial\Omega$ terminate the walk.
(4) Update indexes and coordinates:

$$k \leftarrow k + 1; \qquad t_k \leftarrow t_{k+1}; \qquad \vec{R}_k \leftarrow \vec{R}_{k+1}; \qquad \Omega_k \leftarrow \Omega_{k+1} \tag{4.2}$$

(5) Repeat from step (2) until walk terminates.

Eq (2.2) shows that events (3.1) and (3.2) above are mutually exclusive.

V. USING CARTESIAN PRODUCT SUBDOMAINS

Use of the ideas presented above are substantially advanced by the use of subdomains that are Cartesian products of sets in still lower dimensions. An example is a rectangle, $[x_1 \le x \le x2] \otimes [y_1 \le y \le y2]$ in which the set of points in two dimensions is specified as the Cartesian or outer product ($\otimes$) of two intervals in one dimension. We now consider the use of subdomains Ω_k that are such Cartesian products:

$$\Omega_k = \omega_1(\vec{R}_k) \otimes \omega_2(\vec{R}_k) \otimes \cdots \omega_M(\vec{R}_k) \tag{5.1}$$

The intervals are shown as functions of the interior point $\vec{R}_k$. We might use three one-dimensional intervals to specify a rectangular parallelepiped, or the product of a two-dimensional ring by a one-dimensional interval to get a truncated annulus, or the product of N three-dimensional spheres to describe a finite volume in a $3N$-dimensional space.

The important point is that the diffusion equation in the form Eq (2.5) is separable. That is, if for a lower-dimensional domain ω_l we can find the necessary Green's function (without absorption):

$$\begin{aligned} [-\nabla^2 + \frac{\partial}{\partial t}]g_l(x_l, x_{0l}; t) &= 0; \qquad x_l, x_{0l} \in \omega_l \\ g_l(x_l, x_{0l}; 0) &= \delta(x_l - x_{0l}) \\ g_l(x_l, x_{0l}; t) &= 0; \qquad x_l, x_{0l} \notin \omega_l \end{aligned} \tag{5.2}$$

then

$$G_k(\vec{R}, \vec{R}_k; t) = exp(-U_k t) \prod_l^M g_l(x_l, x_{0l}; t) \tag{5.3}$$

The proof follows by straightforward computation using Eq (5.2).
We also have

$$-\vec{n} \cdot \vec{\nabla} G_0(\vec{R}, \vec{R}_0; t) = exp(-U_k t) \sum_l [-\nabla_{ln} g_l] \prod_{j \neq l} g_l(x_l, x_{0l}; t) \tag{5.4}$$

where $\nabla_{ln} g_l$ denotes the outer normal derivative of $g_l(x_l, x_{0l}; t)$at the boundary of ω_l.
The use of such Green's functions may best be described in a procedural way:

(1) Sample τ_0 from the probability distribution function (pfd) $U_k e^{-U_k \tau_0}$
(2) For $l = 1, \cdots, M$ sample τ_l from the pdf $\int_{\partial\omega_l} [-\nabla_{ln} g_l(x_l, x_{0l}; \tau) dx_l$
(3) Set $t = min(\tau_0, \tau_1, \cdots, \tau_M)$
if $t = \tau_0$ then new $R_k \in \Omega_k$
that is, each x_j is sampled on the interior of its ω_j using $g_j(x_j, x_{0j}; t)$.
else: new $R_k \in \partial\Omega_k$
that is, x_l is put on $\partial\omega_l$, the others on interior points
of their respective domains ω_j.

VI. GREEN'S FUNCTIONS FROM EIGENFUNCTIONS

A practical way of writing down any of the Green's functions cited above is to use eigenfunction expansions. A general approach starts with Green's function defined in Eq(1.2). Consider $\phi_m(\vec{R})$, normalized eigenfunctions of the operator $-\nabla^2 + A(\vec{R})$:

$$[-\nabla^2 + A(\vec{R})]\phi_m(\vec{R}) = \lambda_m \phi_m(\vec{R}) \tag{6.1}$$

Then we may express Green's function for the operator $-\nabla^2 + A(\vec{R}) + \frac{\partial}{\partial t}$ as

$$G(\vec{R}, \vec{R}_0; t) = \sum_m e^{-\lambda_m t} \phi_m(\vec{R}) \phi_m(\vec{R}_0) \tag{6.2}$$

Straightforward application of Eq (6.1) and differentiation with respect to t shows that it satisfies the first line of Eq 1.2. At $t = 0$ it reduces to

$$G(\vec{R},\vec{R}_0;0)=\sum_m \phi_m(\vec{R})\phi_m(\vec{R}_0)=\delta(\vec{R}-\vec{R}_0) \tag{6.3}$$

Expansions for the Green's functions defined in Eq (5.2) can often be written in terms of elementary functions. For example, for a (three-dimensional) sphere of radius a,

$$\phi_m(r)\propto sin(m\pi r/a)/r \tag{6.4}$$

with eigenvalues

$$\lambda_m=\frac{m^2\pi^2}{a^2} \tag{6.5}$$

and Green's function is

$$g(r,t)=\frac{1}{2a^3(r/a)}\sum_{m=1}^{\infty} sin(m\pi r/a)exp(-m^2\pi^2 t/a^2) \tag{6.6}$$

Note that the dimensionless function a^3g depends only on the dimensionless variables $u=r/a$ and $\tau=t/a^2$. This reduces spheres of all possible radii to one case.

The expansion of Eq (6.6) converges slowly at small t. There is a complementary expansion that is in effect an "image" expansion and that converges rapidly at short time. Formally it derives from the Poisson sum rule ([2], p. 275) and it is

$$g(r,t)=\{e^{-u^2/(4\tau)}+\sum_{m=1}^{\infty}[(u+2m)e^{-(u+2m)^2/(4\tau)+(u-2m)e^{-(u-2m)^2/(4\tau)}}]\}/(4\pi\tau)^{3/2} \tag{6.7}$$

Green's function for a one-dimensional interval $[x_1,x_2]$ is similar. Because it is translationally invariant, we need only write it down on some canonical interval, say $-a\le x,x_0\le a$ where it takes the form

$$g(x,x_0;t)=\frac{1}{a}\sum_{m=1}^{\infty} sin[\frac{m\pi(x+a)}{2a}]sin[\frac{m\pi(x_0+a)}{2a}]exp[-(\frac{m\pi}{2a})^2 t] \tag{6.8}$$

Using reduced variables, $u=(x-x0)/a;\tau=t/a^2$ the short-time expansion, corresponding to Eq (6.7) is

$$ag(x,x_0;t)=\sum_{m=-\infty}^{\infty}\frac{e^{-(u+2m)^2/(4\tau)}}{(4\pi\tau)^{1/2}} \tag{6.9}$$

For cylindrical coordinates, we may consider the interval $a\le r\le b$ for which the basis functions are (cf ref [2], p. 206.)

$$\Phi_m(r)=\pi\alpha_m J_0(\alpha_m a)\frac{J_0(\alpha_m r)Y_0(\alpha_m b)-J_0(\alpha_m b)Y_0(\alpha_m r)}{2(J_0^2(\alpha_m a)-J_0^2(\alpha_m b))^{1/2}} \tag{6.10}$$

where $J_0(x)$ is the Bessel function of the first kind of order zero, and $Y_0(x)$ the Bessel function of the second kind of order zero. The eigenvalues are $\lambda_m=\alpha_m^2$ where $\alpha_m q$ are solutions of

$$J_0(\alpha_m a)Y_0(\alpha_m b)-J_0(\alpha_m b)Y_0(\alpha_m a)=0 \tag{6.11}$$

so that the Green's function we need is

$$g_{cyl}(r, r_0; t) = \sum_m e^{-\alpha_m^2 t} \Phi_m(r) \Phi_m(r_0) \tag{6.12}$$

If $b/a - 1$ is not large then

$$\Phi_m(r) \approx [\frac{2}{b-a}]^{1/2} sin[m\pi(r-a)/(b-a)] \tag{6.13}$$

and

$$\alpha_m(r) \approx \frac{a\pi}{b-a} \tag{6.14}$$

This can be used very well as the starting point for a rapidly converging iterative solution of Eq (6.11). Also, Eq (6.14) means that for most zones, computation with sines and cosines can replace use of the Bessel functions.

VII. SAMPLING THE FUNCTIONS

We need to consider how to sample new positions and time intervals from $g_l(x_l, x_{0l}; t)$ and $\int_{\partial\omega_l}[-\nabla_{ln} g_l(x, x_{0l}; t)]dx$, respectively. As a basis for experimentation, we prepared robust but not optimally efficient routines for the purpose. For the positions in the interior of the subdomains, we used rejection techniques based the leading terms of the short and long time expansions. For sampling times to boundary absorption, we proceed as follows: Denote

$$H_l(t) = \int_{\omega_l} g_l(x, x_{0l}; t)dx \tag{7.1}$$

It follows from Eq(5.2) that

$$H_l'(t) = \int_{\omega_l} \frac{\partial g_l(x, x_{0l}; t)}{dt} dx; \tag{7.2}$$

$$= -\int_{\partial\omega_l} \nabla_{ln} g_l(x, x_{0l}; t)dx. \tag{7.3}$$

It is straightforward to compute $H_l(t)$ (in appropriate dimensionless form) from sort or long time series and to tabulate the results in a form straightforward to sample. These routines exist in usable form. They have been tested using soluble test problems. They have not been tested in the context of radiation transport. The plan is to test the efficiency of the calculation when the sphere construction presently used is replaced by rectangular and/or cylindrical domains. The expectation is that the better fit of the new shapes now available will speed up the calculations. This will be very much application dependent. On the other hand, the use of boxes or cylinders is somewhat more expensive, requiring sampling for each of the orthogonal directions, and more complicated geometry to orient the subdomain. It may be that a speedup will be attained only when the existing routines are made more efficient, but there is significant room to do that.

REFERENCES

[1] M.H. Kalos, D. Levesque, and L. Verlet, "Helium at Zero Temperature with Hard Sphere and Other Forces", Physical Review A 9 (1974).

[2] H.S. Carslaw and J.C. Jaeger, "Conduction of Heat in Solids", Clarendon Press, (Oxford, 1959), p. 275.

Although this term could be made small by choosing $\Delta\tau$ small enough, we do not do so in order to find the "worst case scenario." Hence, ignoring $1/\Delta\tau$,

$$\begin{aligned} \lim_{(c\Delta t)\to 0} \Delta S_i &< +p \,/\, c_{\mathrm{v},i} \\ &= (S_i'/\bar{S}_i')\,(\bar{c}_{\mathrm{v},i}/c_{\mathrm{v},i})\,(S_0 - S_i) \\ &< (S_i'/\bar{S}_i')\,(\bar{c}_{\mathrm{v},i}/c_{\mathrm{v},i})\,S_0 \,. \end{aligned} \tag{40}$$

Since $\bar{S}_i'$ is obtained at an intermediate point between S_0 and S_i, $(S_i'/\bar{S}_i') < 1$. For an ideal gas, $\bar{c}_{\mathrm{v},i}/c_{\mathrm{v},i} = 1$; hence, $\Delta S_i < S_0$. As long as $c_{\mathrm{v},i}$ grows no faster than T^3, we still get $(S_i'/\bar{S}_i')\,(\bar{c}_{\mathrm{v},i}/c_{\mathrm{v},i}) \leq 1$ and the lemma is proved.[1] To summarize, we stress that the condition $\Delta S_i < S_0$ is a worst case. Under normal conditions, we expect $\Delta S_i < 0$ as desired. ▌

Because the iterates satisfy a discretization of (24), the densities E_i and $\rho\, e_i$ satisfy a conservation law. It is easy to see what contributes to the radiation energy change, $V\,(E_{i+1} - E_i)$, for each iterate in each cell. In particular the term,

$$\Delta\tau\,[\,\mathcal{K}\,(S - E)\,]_{i+1} \doteq \Delta\tau\,[\,\mathcal{K}_i\,(S_{i+1} - E_{i+1}) + \mathcal{K}_i'\,(S_i - E_i)\,(S_{i+1} - S_i)\,] \tag{41}$$

is the energy transferred from the matter. In that light, energy is conserved by setting,

$$e_{i+1} = e_i + \Delta\tau \left\{ e_0 - e_i - \frac{c_{\mathrm{v},i}}{S_i'}\,(S_{i+1} - S_i) - [\,\mathcal{K}\,(S - E)\,]_{i+1} \right\} , \tag{42}$$

where the coupling term is defined in (41). If (42) should ever yield $e_{i+1} < 0$, we easily recover by using the EOS: $e_{i+1} = e(T_{i+1})$ where $T_{i+1} = (S_{i+1}/a)^{1/4}$.

We conclude the Ψtc analysis with two more items.

4.1 Ψtc for large Δt

Setting the real time step Δt very large effectively discards the first term on the rhs of (10) and (11). In this case, the Ψtc iterations are very robust. Equation (28) becomes,

$$-\mathcal{D}_i\,E_{i+1} + (\,V/\Delta\tau + \alpha_i\mathcal{K}_i\,)\,E_{i+1} = (V/\Delta\tau)\,E_i + \alpha_i\mathcal{K}_i S_i \,,$$

while (29) becomes,

$$S_{i+1} = (1 - \gamma_i)\,S_i + \gamma_i\,E_{i+1} \,,$$

where α_i and γ_i are defined as before, but now $a_i = m\,c_{\mathrm{v},i}\,V/\Delta\tau$. Clearly, there is no danger of unphysical iterates.

However, in most applications, even though Δt may be large, the two terms on the rhs of (11) may be comparable, especially if the temperatures are cold. For example, for hydrogen, if T is measured in keV, $e = 0.1\,T$ while $E \approx S = 0.0137\,T^4$. Hence, we should also analyze the effects of only discarding $\partial_t E$. In this regime, on the lhs of (28), $g_i \to V/\Delta\tau + \alpha_i\mathcal{K}_i$ while on the rhs the term $V\,E_0$ is discarded. Equation (29) and the definitions (27) are unchanged. The previous analysis holds, but $\Delta\tau$ might be restricted further because on the rhs of (28), which must still be kept positive, we lose the term $V\,E_0$. Also, the system is less diagonally dominant because g_i is smaller. Nevertheless, $\Delta\tau$ still exerts a stabilizing effect on the iterations.

4.2 Conclusion of Ψtc iterations

In a sense, determining when to stop iterating is trivial. The answer is obtained when $S_{i+1} = S_i$ and $E_{i+1} = E_i$. However, in order to have an efficient termination criterion, we focus attention on when the matter energy stops changing. First, we compute the maximum energy in a cell, at the i^{th} step

$$(me)_{i,x} = \max_{\text{cells}} (m\,e_i)$$

[1] For the Pomraning problem, since $c_{\mathrm{v},i} \propto T^3$, $(S_i'/\bar{S}_i')\,(\bar{c}_{\mathrm{v},i}/c_{\mathrm{v},i}) = 1$.

and stop whenever

$$\frac{m\,(e_i - e_{i-1})}{m\,e_i + \epsilon_1\,(me)_{i,x} + \epsilon_2\,(me)_0} < \epsilon_3\ , \tag{43}$$

where $(me)_0$ is a user-specified reference energy and the ϵ_i are user specified parameters. The criterion halts the iterations if either the relative energy change, or two comparisons of the absolute change are small. Suggested values are $\epsilon_1 = \epsilon_2 = 0.001$ and $\epsilon_3 = 10^{-8}$.

Of course, halting when the matter energy has converged is not the whole story, but typically the matter energy is larger than the radiation energy. Nevertheless, if (43) is satisfied at the i^{th} step, the next iteration for E_{i+1} is (28) where we explicitly write $\mathcal{D}_i = \mathcal{D}(E_i,\, S_i)$ to show that the diffusion coefficient depends on both E_i and S_i. If we now assume that $S_{i+1} = S_i$, then $e_{i+1} = e_i$ and the previous iteration is of the form,

$$-\mathcal{D}(E_{i-1},\, S_i)\,E_i + g_i\,E_i = (V/\Delta\tau)\,E_{i-1} + V\,E_0 + \alpha_i \mathcal{K}_i S_i + (1-\alpha_i)\,m\,(\,e_0 - e_i\,)\ , \tag{44}$$

Subtracting (44) from (28) yields,

$$-[\,\mathcal{D}(E_i,\, S_i)\,E_{i+1} - \mathcal{D}(E_{i-1},\, S_i)\,E_i\,] + g_i\,\Delta E_i = (V/\Delta\tau)\,\Delta E_{i-1}\ , \tag{45}$$

where $\Delta E_i = E_{i+1} - E_i$. The different diffusion coefficients stem from the flux limiter. This difference may be ignored since the flux limiter is only a kludge. After dividing by γ_i, (45) becomes

$$-(1/g_i)\,\mathcal{D}_i\,\Delta E_i + \Delta E_i = h_i\,\Delta E_{i-1}\ .$$

where $0 < h_i = (V/\Delta\tau)/g_i < 1$. This is an elliptic equation with homogeneous boundary conditions. The rhs is a fraction of what is presumably already a small quantity ΔE_{i-1}. Hence, ΔE_i is smaller yet and the E equation may also be deemed to have converged.

If by chance we halted prematurely, there is one more control available. If (24) is viewed as a system of evolution equations, the coefficients have "characteristic times" that govern how long (in pseudo time) it takes to equilibrate. If (24) is divided by the cell volume V, the units are energy-density/pseudo-time. If τ is the approximate time to equilibrate, then from the e equation and the absorption term, $e/\tau \approx -e$ which yields $\tau \approx 1$. Similarly, from the coupling term,

$$m\,e/\tau \approx \mathcal{K}\,S = c\,\Delta t\,m\,\kappa\,S$$

which yields,

$$\tau \approx e/(c\,\Delta t\,\kappa\,S)$$

as another estimate for how long (in pseudo time) to iterate.

5 Pomraning Problem

We now present results on the Pomraning problem, [2] and [3], which simulates a radiation wave propagating into cold material. After some algebra, for this problem, the equations may be put in the form,

$$\partial E/\partial\tilde{t} = \nabla\cdot D\nabla E + (1/\epsilon)\,(S - E) \tag{46}$$

$$\partial e/\partial\tilde{t} = -(1/\epsilon)\,(S - E)\ . \tag{47}$$

where $D = 1/(3\,\epsilon)$, $e = S/\epsilon$, and $S = aT^4$. The term ϵ is a constant which arises by using $c_{\rm v} = c_{{\rm v},0}T^3$ and setting $\epsilon = 4a/c_{{\rm v},0}$. In (46)-(47), $\kappa = \rho = 1$. Hence, $e = \rho e$ is now the internal energy density. The normalized time $\tilde{t} = \epsilon\,c\,\kappa\,t$.

The specifications of the Pomraning problem dictate $S \le E$. Since (46)-(47) imply that ϵ is an approximate time for the fields to equilibrate, it is interesting to examine what happens at early times using the backward Euler ($\theta = 1$), semi-implicit scheme described in §2. Table 1 displays the energy

$\Delta\tilde{t}_0$	$\tilde{t}$	$j=0$	1	2	3	4
1.e-7	1.e-7	-1.5e+7	-1.6e-3	9.4e-10	2.5e-12	6.1e-15
1.e-8	1.e-8	-1.5e-1	3.2e-8	9.6e-13	2.6e-16	6.2e-20
1.e-9	1.14e-8	1.1e-5	2.4e-9	3.4e-13	3.6e-17	3.1e-21
1.e-10	1.09e-8	1.1e-5	2.0e-9	2.4e-13	2.1e-17	1.4e-21

Table 1: Energy exchange term $E_i - S_i$ for the Pomraning problem. First and second columns denote the initial time step and current time resp. Simulation uses $\epsilon = 0.1$

exchange term $E_j - S_j$ where j denotes the mesh index. A nonuniform mesh is used; $\Delta z_0 = 0.01$, and for $j > 0$, $\Delta z_j = \Delta z_0\,(1.05)^j$. The table shows that for $\Delta\tilde{t}_0 = 10^{-8}$, at the incident edge, $S_0 > E_0$ violating the physics. For larger $\Delta\tilde{t}_0$, the result is even worse, e.g., if $\Delta\tilde{t}_0 = 10^{-6}$, after one cycle, $E_0 - S_0 = -1.2 \cdot 10^{15}$

We note that the above error does not occur for the proposed Ψtc scheme. However, the lack of the error is *not* due to the introduction of the pseudo-temporal derivative, but is instead due to iterating on S instead of T. Indeed, since the opacity κ is constant, for the first iteration, the pseudo-time step $\Delta\tau$ is not restricted; hence, $1/\Delta\tau = 0$. Equation (34) still holds and for the first time step of the Pomraning problem, it reduces to,

$$S_1 = \gamma_0 E_1 \quad \gamma_0 = 1/(1 + \alpha_0 \mathcal{K}_0/V)\ ,$$

where the subscripts now denote the iteration number and where $\alpha_0 = 1/(1 + c\Delta t\kappa\epsilon) = 1/(1 + \Delta\tilde{t})$. This is the desired behavior; viz., $S_1 \leq E_1$ with equality obtained only as $\Delta\tilde{t} \to \infty$.

Iterating on S (instead of T) is the cause of the good fortune. Substituting $\Delta T = \Delta S/S_0'$ into (8) yields

$$\lim_{\Delta t\to\infty} \Delta T = \lim_{\Delta t\to\infty} \Delta S/S_0' = (E - S_0)/S_0'\ ,$$

and we obtain $S = E$ as desired.

The analysis is easily extended to other problems with more general material properties, e.g., $c_v = c_{v,0}T^\beta$ and $\kappa = \kappa_0 T^\delta$. The moral is that since $S \propto T^4$, it is better to solve for (and iterate on) what varies rapidly (S), then take its fourth root (to get T) instead of using T and then taking its fourth power.

6 Conclusion

We have developed a scheme to solve the nonlinear system of equations describing radiation diffusion coupled to matter energy balance. Because of the nonlinearities, iterations are required. After multiplying by the time step Δt, the equations mimic a coupled system with transport, explicit sources and absorption. By introducing Ψtc, the system is solved when the (pseudo-time) steady state is reached. Each iteration is a temporal advance in pseudo-time and requires only one solve of a scalar elliptic equation. The scheme is robust; by controlling the pseudo-time step $\Delta\tau$, each iterate is guaranteed to be positive and bounded by the previous iterate and the boundary conditions. The solution is first order accurate in (real) time. Arbitrarily large Δt's are allowed. Upon convergence, all of the coefficients are evaluated at the advanced time level.

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